

Backward non-unitary quantum evolution

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Abstract

A non-linear backward equation with diffusive terms is postulated for the probability density that depends on the Bohmian quantum potential. An associated nonlinear Schrödinger equation is also introduced and extension of the analysis to several particle compounds is sketched along with the implications following from this formalism regarding the non-conservation of probability in the non-equilibrium regime. Some further conclusions are deduced with respect to the Onsager's relations and the generalized optical theorem.

In one of the early papers on wave mechanics, Darwin [1, 2] examined an interesting example of a two-particle quantum interference involving a set up of a coherent pair of particles. A few years later interparticle quantum correlations between two bodies became notable with the work of Einstein, Podolsky and Rosen[3, 4] and since then have been at the heart of quantum mechanics. The issue of non-separability between interacting particles had been particularly emphasized by Einstein in his own version of the EPR thought experiment [5]. Schrödinger in a similar vein claimed quite succinctly that according to quantum theory maximum knowledge of a composite system does not necessarily mean fullest knowledge of the individual particles [6, 7]. This type of reasoning that emphasizes the influence of the particular experimental conditions for the available type of possible predictions has been extensively used by Bohr in his reply to Einstein-Podolsky-Rosen [4] and is best illustrated in the ingenious thought experiments devised earlier by him and Rosenfeld for the measurability of fields [8]. More recently Mermin in particular emphasized the physical reality of these subsystem correlations in comparison to the *correlata* underlying them. From a rather different perspective, the quantum potential which has a pre-eminent role in Bohmian dynamics, is associated with the interrelatedness in the quantum world and suggests a quality of irreducible wholeness in the domain

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of quantum phenomena [10, 11]. Here we will modify the continuity equation for the probability density by including a term proportional to the quantum potential and examine some of its consequences.

Another issue that needs to be addressed is the time asymmetry observed in the physical world in contradistinction to the time symmetrical form of the fundamental equations of evolution [12]. The resolution of the contradiction in classical mechanics is usually related to an asymmetry in initial conditions. In quantum mechanics in particular, Schrodinger equation becomes time reversible if we make the identification of the probability amplitude with the time symmetrical complex conjugate one. It is generally appreciated that the quantal irreversibility is the result of initial conditions or the outcome of the interaction of a few particle system with a reservoir but recently it has been shown experimentally [13] that even a few particles may exhibit signs of irreversibility. The collapse of the wavefunction on the other hand is generally accepted to impose a genuinely time asymmetric element in the quantum formalism.

In this work we follow a different approach, by demonstrating that the quantum potential term mentioned above may be employed in a way that implies that the evolution equation for the probability density is genuinely time-asymmetric. It deserves notice that the equation that will be proposed depends on a final value condition so it turns out to be backward [14] and resembles on that respect the Kolmogorov backward equation [15], the adjoint transport equation [16] or the Black-Scholes one known from mathematical finance [17]. Following this we extend our study for the multiparticle and present some conclusions related to the quantum equilibrium hypothesis, Onsager's relations, the generalized optical theorem and finally we recapitulate our findings in the final section.

Generalized continuity equation and its associated non-linear wave equation. In a recent paper [18] it has been argued that quantum theory may not be extended straightforwardly to the macroscopic domain. This could lead us to seek generalizations of the present quantum formalism. Since standard non-linear versions of the Schrodinger equation [19, 20] seem to face certain difficulties [21] we try instead to generalize the Bohmian-de Broglie formulation. Employing the position representation, we consider initially a neutral, spinless particle of mass m , assuming that the time varying potential is $V(t)$. The fundamental quantum mechanical equation of motion for the single particle probability amplitude reads as

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi. \quad (1)$$

The familiar polar substitution $\Psi = R e^{iS/\hbar}$ gives the Hamilton-Jacobi-Madelung equation when we equate the real parts

$$\frac{\partial S}{\partial t} = \frac{\hbar^2}{2m} \left[\frac{(\nabla^2 R)}{R} - \frac{1}{\hbar^2} (\nabla S)^2 \right] - V. \quad (2)$$

We may also define the quantum potential as

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}, \quad (3)$$

which is important in Bohm's version of the de Broglie-Bohm mechanics, although it is possible to formulate the theory without any reference to it. Equating the imaginary parts we obtain

$$\frac{\partial R}{\partial t} + \frac{1}{2m} (2\nabla R \cdot \nabla S + R\nabla^2 S) = 0. \quad (4)$$

Born's rule which at least in text-book quantum mechanics is considered a separate axiom of quantum physics provides a conceptual and calculational bridge between theory and experimental results. Taking into account then the identification $\rho = u^2$ for the probability density and multiplying both sides with $2u$ yields the familiar continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = 0. \quad (5)$$

From (2) and (4) we may determine in principle the action S and the amplitude R . We seek to modify the previous expression (4) including a diffusion term and a linear term proportional to the quantum potential as follows

$$\frac{\partial u}{\partial t} + \frac{1}{2m} (2\nabla u \cdot \nabla S + u\nabla^2 S) = \left(-\frac{\hbar}{2m} \right) \left(\nabla^2 u - \frac{\nabla^2 R}{R} u \right). \quad (6)$$

This formula may be considered as a non-equilibrium extension of (4) in the sense that as $u \rightarrow R$ the former reduces to the familiar equation that holds at quantum equilibrium. The given expression remains time-asymmetrical which immediately implies non-unitary evolution (the inverse proposition is not true nevertheless). The negative coefficient suggests a backward evolution for $u(t)$. We conclude then that not only the evolution equation is not time-invariant but that also there is time asymmetry in the imposition of terminal instead of initial conditions. An element then of finality is introduced in (6) since it relies on terminal values evolving backwards in time. The homogeneity condition is satisfied since for an arbitrary solution u and κ a real number it follows immediately that κu is also a solution. Hence the rescaling transformation $u' \rightarrow \kappa u$ constitutes a similarity transformation that leaves the equation invariant. An imaginary quantum potential would give rise to dissipative terms that do not preserve unitarity in the general case. At the same time we must ensure that the expression reduces to the standard form at equilibrium. This suggests an extension of (1) written as

$$i\hbar \frac{\partial \Phi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Phi - i\frac{\hbar^2}{2m} \left(\frac{\nabla^2 \sqrt{|\Phi|^2}}{\sqrt{|\Phi|^2}} - \frac{\nabla^2 \sqrt{|\Psi|^2}}{\sqrt{|\Psi|^2}} \right) \Phi. \quad (7)$$

where $\Phi = ue^{iS/\hbar}$ and the wavefunction $\Psi = Re^{iS/\hbar}$ is governed by (1) with appropriate final conditions. The existence of a distinct wave function with

the same phase as Ψ but different real amplitude is reminiscent of the double solution theory put forward by de Broglie [22], but it must be noted that in (7) Φ propagates backward in time in the configuration space in the same manner as Ψ , so it is not a singularity in the real three dimensional space as de Broglie envisaged. Dynamical terms of the form given in (7) have also been used in the past in the real but not in the imaginary part of the Hamiltonian [23]. It must be underscored that when the terminal condition is fulfilled, which means $u(t \rightarrow \infty) = R(t \rightarrow \infty)$ so $\Phi(t \rightarrow \infty) = \Psi(t \rightarrow \infty)$ the superposition principle holds and we recover (1) from (7) even though the coefficient \hbar/m is obviously different from zero. Hence the magnitude of the non-linearity coefficient may be non-zero nevertheless there is an appropriate limit that we recover (1). On the other hand a nonlinear Schrödinger as in [19] reduces to the linear one only when the nonlinearity constant becomes zero. Finally, (7) is time irreversible even when $\Phi \rightarrow \Phi^*$ and respects the homogeneity condition [20] which says that if Φ is a solution of (7) so is $\Phi \rightarrow Z\Phi$, where Z a constant complex number. Based on (7) we can present extensions of standar quantum formulas. If we write for example the expectation value of an operator \hat{A} as

$$\langle \hat{A} \rangle = \int \Phi^* \hat{A} \Phi d^3x, \quad (8)$$

its time development is given by

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle - \frac{\hbar}{m} \mathbf{Re} \int \Phi^* \left(\frac{\nabla^2 \sqrt{|\Phi|^2}}{\sqrt{|\Phi|^2}} - \frac{\nabla^2 \sqrt{|\Psi|^2}}{\sqrt{|\Psi|^2}} \right) \hat{A} \Phi d^3x \quad (9)$$

where \hat{H} the Hamiltonian and of course the first two terms make up the familiar expression in the Schrödinger picture whereas the last term reflects dissipative effects. According to (6) and taking into account that $\rho = |\Phi|^2$, the corresponding expression for the probability density is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = \left(-\frac{\hbar}{m} \right) \left[\frac{1}{2} \nabla^2 \rho - \frac{(\nabla \rho)^2}{4\rho} - \frac{\nabla^2 R}{R} \rho \right]. \quad (10)$$

The left part is familiar from the continuity equation but the right non zero part implies non-unitary evolution. The existence of these terms suggests a possible interplay between spatial-temporal coherence and diffusion phenomena. Diffusion terms in the continuity equation have been also been added in [24, 25] (see also [26, 27]). In addition equation (10) remains invariant when $R \rightarrow \kappa R$ and $\rho \rightarrow \lambda \rho$. It must be noted though that the diffusion constant in our proposal is negative, namely $-\hbar/m$ as we mentioned. Without the the nonlinear and the quantum potential term, (10) is a non-equilibrium backward Fokker-Planck type equation that conserves probability locally. The inclusion of the quantum potential and nonlinear terms destroy this property and is responsible for its non-conservation. It is evident that superluminal communication is precluded by the very fact that the relevant equation of motion for the probability density

depends on the imposition of a final condition. This preferential status of terminal conditions instead of initial means that we could use (6),(7), or (10) to make retrodictions but not predictions. It may be commented that this special importance of final conditions can be clearly illustrated with the help of the well-known thought delayed choice experiment [28] and even the Bohrian emission of photons during atomic transitions in the old quantum theory era. At the equilibrium limit these reduce to the more familiar Bohmian equations so they may be seen as generalizations of the latter in the non-equilibrium domain. The presence of the diffusion terms would tend to make u smoother but the quantum potential driving term and especially the highly nonlinear midterm could have the opposite effect. On physical grounds we would expect irregularities in $\rho(x, t)$ to become less smooth with backward time evolution which may cause problems for the behaviour of the solutions like arbitrary rapid growth in finite time [14]. The presence then of the nonlinear terms is of special importance, since if they tend to create irregularities as we propagate backwards in time and dominate over the decay term that will decide in favour of the ill-posedness of the problem and would demand sophisticated regularization techniques. Obviously, we could also include advanced vector potentials and even noise terms in (10) [29]. The latter ones require special care though because of certain mathematical subtleties involved [30].

It must be emphasized though that there are no non-intersecting particle trajectories apart from the case of equilibrium when (8) becomes the familiar density current equation and the coefficient sets time scale equal to \hbar/m . We now seek a guidance equation modifying the de Broglie-Bohm one. Motivated by (11) we write a formula for the velocity \mathbf{v} of a single particle that would accompany (7) as

$$\mathbf{v} = \frac{\hbar}{m} \mathbf{Im} \frac{\Phi^* \nabla \Phi}{|\Phi|^2} - \frac{\hbar}{2m} \left[\nabla \ln |\Phi|^2 - \frac{1}{|\Phi|^2} \int d^3x \left(\frac{(\nabla |\Phi|^2)^2}{2|\Phi|^2} + \frac{2|\Phi|^2 \nabla^2 \sqrt{|\Psi|^2}}{\sqrt{|\Psi|^2}} \right) \right]. \quad (11)$$

The first term in the above formula is the velocity term $\frac{\nabla S}{m}$, the second one proportional to $\nabla \ln |\Phi|^2$ is an osmotic type contribution to velocity according to [10, 31, 32] (note the negative sign of the diffusion coefficient) and the third integral term expresses the non-local character of this generalized guidance equation and clearly violates the uniqueness property of trajectories. Since the last two term cancel each other when $\Phi = \Psi$ we recover the standard guidance equation. Having established the basic elements of the formalism (relevant evolution equations) we proceed by examining some further developments and examples.

It is interesting to note, as it is clearly seen in (10) or (11), that even when the gradient of the action is zero, the probability density may be nonstationary which implies the possibility of backflow effects. The inverse is also true, (10) allows a steady state density even when the the momentum is non-zero. Since \hbar/m is very small we expect that these deviations from (5) to be very weak. Seeking a similarity solution we proceed by defining the scaling *ansatz* $\eta = \frac{x}{\sqrt{\frac{\hbar}{m} t}}$

and obtain a nonlinear ordinary differential equation which still may be not amenable to analytic solution. Instead we could make the substitution $\rho = e^{2h}$ to (10) when the spatial derivative of the phase is considered negligible and find

$$\frac{\partial h}{\partial t} = \left(-\frac{\hbar}{2m}\right) \left[\nabla^2 h + (\nabla h)^2 + \frac{2m}{\hbar^2} Q \right]. \quad (12)$$

The above resembles the celebrated Kardar-Parisi-Zhang equation [33] that has many applications in the field of surface growth. The crucial difference is that it propagates backward in time and the last quantum potential driving term should be considered deterministic in general instead of stochastic.

Non-conservation of total probability and entropy production rate. The rate of change of the total probability is expressed as

$$\frac{dP}{dt} = \frac{d}{dt} \int d^3x \rho = \int d^3x \frac{\partial \rho}{\partial t} = \left(-\frac{\hbar}{m}\right) \int \left[\frac{1}{2} \nabla^2 \rho - \frac{(\nabla \rho)^2}{4\rho} - \frac{\nabla^2 R}{R} \rho \right] d^3x. \quad (13)$$

The second term makes apparent a connection to Fisher information, which is a measure of system disorder [34, 35]. As ρ approaches R the rate of change of the total probability becomes zero. Making use of the identities $\frac{\nabla R}{R} = \nabla \ln R$ and $\frac{\nabla^2 R}{R} = \nabla^2 \ln R + (\nabla \ln R)^2$ and allowing $\rho \rightarrow R^2 + \delta\rho$, the variation of the total probability rate δI may be written as

$$\delta I = \left(-\frac{\hbar}{m}\right) \int d^3x \left(\frac{1}{2} \nabla^2 - \nabla \ln R \nabla - \nabla^2 \ln R \right) \delta \rho. \quad (14)$$

Differentiating over time the Gibbs entropy $G = - \int d^3x \rho \ln \rho$ which relies on the spatial distribution of the probability density gives the following rate for the production of entropy

$$\frac{dG}{dt} = - \int d^3x \left(\nabla \rho \frac{\nabla S}{m} \right) + \frac{\hbar}{m} \int d^3x (1 + \ln \rho) \left[\frac{1}{2} \nabla^2 \rho - \frac{(\nabla \rho)^2}{4\rho} - \frac{\nabla^2 R}{R} \rho \right]. \quad (15)$$

The second integral remains unaffected when time is reversed and can be identified as a measure of entropy production Σ and a sign of system irreversibility. The other term in (15) is associated with entropy flow that follows from (5). Again near the linear approximation regime $\rho \rightarrow R^2 + \delta\rho$ the variation of entropy production is given by

$$\delta \Sigma = \sum_{i,j} \nabla F_i L_{ij} \nabla F_j. \quad (16)$$

In the last equality, $F_{i,j}$ are generalized thermodynamical forces near equilibrium [36] and L_{ij} the corresponding Onsager coefficients. Since microscopic time reversibility and the resulting detailed balance do not hold it follows according to (15),(16) that these coefficients may not be symmetrical.

Quantum scattering and the generalized optical theorem. Up to this point we have only considered time dependent evolution equations. It is possible nevertheless to make use of a time-independent version of (7) invoking its imaginary potential. The time-independent variant of this nonlinear wave equation for a particle with energy E , mass m and wave-vector \mathbf{k} is written as

$$\left[(\nabla^2 + k^2 - U_r) - i \left(\frac{\nabla^2 \sqrt{|\Phi(\mathbf{r})|^2}}{\sqrt{|\Phi(\mathbf{r})|^2}} - \frac{\nabla^2 \sqrt{|\Psi(\mathbf{r})|^2}}{\sqrt{|\Psi(\mathbf{r})|^2}} \right) \right] \Phi(\mathbf{r}) = 0 \quad (17)$$

where $k = \sqrt{2mE}$, $U(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r})$ and $V(\mathbf{r})$ a central potential. When $\Phi(\mathbf{r}) = \Psi(\mathbf{r})$ the formal solution of (17) can be written as

$$\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \int G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \Psi(\mathbf{r}') d^3x \quad (18)$$

where $G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}')$ the corresponding Green function and $\Psi_0(\mathbf{r})$ a solution of the homogeneous equation $(\nabla^2 + k^2)\Psi_0(\mathbf{r}) = 0$ [37]. Due to the nonlinear character of (17) it is not possible to write a relation similar to (18) for $\Phi(\mathbf{r})$. We can proceed though by assuming that at large distances from the potential region the solution $\Phi(\mathbf{r})$ has the asymptotic form

$$\Phi_{\mathbf{k}} \rightarrow e^{i\mathbf{k} \cdot \mathbf{r}} + \frac{e^{ikr}}{r} f(\mathbf{k}, \mathbf{k}'). \quad (19)$$

Following the analysis by Glauber [38, 37] for two scattering vectors \mathbf{k}, \mathbf{k}' (17) produces the identities

$$\Phi_{-\mathbf{k}'} \nabla^2 \Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'} \nabla^2 \Phi_{-\mathbf{k}} = 0 \quad (20)$$

and

$$\nabla \cdot [\Phi_{\mathbf{k}'}^* \nabla \Phi_{\mathbf{k}} - \Phi_{\mathbf{k}} \nabla \Phi_{\mathbf{k}'}^*] + 2i \left(\frac{\nabla^2 \sqrt{|\Phi_{\mathbf{k}}|^2}}{\sqrt{|\Phi_{\mathbf{k}}|^2}} - \frac{\nabla^2 \sqrt{|\Psi_{\mathbf{k}}|^2}}{\sqrt{|\Psi_{\mathbf{k}}|^2}} \right) \Phi_{\mathbf{k}'}^* \Phi_{\mathbf{k}} = 0 \quad (21)$$

Integrating (20) and using Green's theorem over the volume of a very large sphere gives $f(\mathbf{k}', \mathbf{k}) = f(-\mathbf{k}', -\mathbf{k})$ which expresses the reversibility of the scattering processes/amplitudes for two directions [38]. Furthermore, if the scattering potential has inversion symmetry then the scattering amplitude is symmetric $f(\mathbf{k}', \mathbf{k}) = f(\mathbf{k}, \mathbf{k}')$ which is clearly related to the principle of detailed balance [38]. This conclusion nevertheless does not contradict our previous discussion which relied on a time-dependent evolution equation. Following the same procedure for (21) we find

$$\begin{aligned} \frac{1}{2i} [f(\mathbf{k}', \mathbf{k}) - f^*(\mathbf{k}, \mathbf{k}')] &= \frac{k}{4\pi} \int f^*(\mathbf{k}'', \mathbf{k}) f(\mathbf{k}'', \mathbf{k}) d\Omega_{\mathbf{k}''} \\ &- \frac{1}{4\pi} \int \left(\frac{\nabla^2 \sqrt{|\Phi_{\mathbf{k}}|^2}}{\sqrt{|\Phi_{\mathbf{k}}|^2}} - \frac{\nabla^2 \sqrt{|\Psi_{\mathbf{k}}|^2}}{\sqrt{|\Psi_{\mathbf{k}}|^2}} \right) \Phi_{\mathbf{k}} \Phi_{\mathbf{k}'}^* d^3x. \end{aligned} \quad (22)$$

Setting $\mathbf{k} = \mathbf{k}'$ gives

$$\text{Im}f(\mathbf{k}, \mathbf{k}') = \frac{k}{4\pi}\sigma_{sc} - \frac{1}{4\pi} \int \left(\frac{\nabla^2 \sqrt{|\Phi_{\mathbf{k}}|^2}}{\sqrt{|\Phi_{\mathbf{k}}|^2}} - \frac{\nabla^2 \sqrt{|\Psi_{\mathbf{k}}|^2}}{\sqrt{|\Psi_{\mathbf{k}}|^2}} \right) |\Phi_{\mathbf{k}}|^2 d^3x. \quad (23)$$

The integrand in the right hand of (22) is easily identified with the divergence of the current density $\mathbf{j} = |\Phi_{\mathbf{k}}|^2 \frac{\nabla S}{m}$. Writing $\Phi_{\mathbf{k}} = e^{g(\mathbf{r})} \Psi_{\mathbf{k}}$ (since they both have the same phase) where $g(\mathbf{r})$ an unknown real function to be determined yields the integral equation

$$4\pi \text{Im}f(\mathbf{k}, \mathbf{k}') = k\sigma_{sc} - \int \left[\nabla^2 g(\mathbf{r}) + \nabla g(\mathbf{r}) \cdot \nabla \ln \sqrt{|\Psi_{\mathbf{k}}|^2} + (\nabla g(\mathbf{r}))^2 \right] e^{2g(\mathbf{r})} |\Psi_{\mathbf{k}}|^2 d^3x. \quad (24)$$

It is clear that we recover the optical theorem for elastic scattering when $\Phi_{\mathbf{k}} = \Psi_{\mathbf{k}}$ which it is known that expresses the particle conservation requirement but more generally deviations may be observed according to (23) or (24). When the above quantity is positive attenuation of the incident beam is implied. It is interesting to note that the presence of the imaginary potential in (17) introduces non-unitarity since the total particle number is not conserved, but does not affect the reversibility of the scattering amplitude [38].

Many particle case and conclusions. It is straightforward to extend our previous results for the case of a compound of several interacting particles of equal masses m

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^N \nabla_i \cdot \left(\rho \frac{\nabla_i S}{m} \right) = \left(-\frac{\hbar}{m} \right) \sum_{i=1}^N \left[\frac{1}{2} \nabla_i^2 \rho - \frac{(\nabla_i \rho)^2}{4\rho} - \frac{\nabla_i^2 R}{R} \rho \right]. \quad (25)$$

The presence of the many particle quantum potential in the continuity equation signifies an important feature, namely the dependence of the multiparticle density on a quantity that exhibits non-local characteristics (but since (25) is backward in time there is no possibility of non-local signalling). The interconnectedness of the system constituents is expressed then through the form of this non-local quantum potential. The constituent particles then are reidentified and incorporated into a substantial whole unified by a single unifying principle and cannot be considered as distinct aggregated components. This means that the component parts even though are retrievable in principle, they are not intrinsically unaffected by their union [39, 40, 41]. Similar considerations in a broader sense have also been expressed various authors. Whitehead for example has spoken about the concept of a dynamic and contextual organic whole [42], as of course Bohm and Hiley [43, 44] already mentioned.

In summary, in the present genuinely multiparticle formulation ontological priority is given not to the monadic particle but to the emergent several-particle composite. We conclude that the presence of the many particle quantum potential in the modified backward continuity equation suggests non-separability

and illustrates the irreducible nature of a multi-particle compound. It is reasonable to deduce then that we cannot examine each particle *singulatim* neither we should consider the quantal multiparticle as a mere mereological aggregate of distinct co-present entities accidentally unified, but rather as a substantial unified whole that constitutes the production of a new physical reality. This particular formalism also ensures that the time anisotropy inferred from the evolution equation and its dependence on terminal values is nomological and intrinsic in nature rather than contingent and accidental.

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